Denmak, Odense, Denmark; [2]Odense University Hospital &Medical Biotech Center, Odense, Denmark; [3]Max Planck Institute for Biochemistry, D Martinsried, Germany; [4]University of Copenhagen, Denmark

MOG pm 2:50 **Activity Dependent Changes in Synaptic Composition**; Jonathan C. Trinidad[1]; Agnes Thalhammer[2]; Aenoch Lynn[1]; Peter Baker[1]; Ralf Schoepfer[2]; A.L. Burlingame[1]; *[1]University of California, San Francisco, San Francisco, CA; [2]University College London, London, UK*

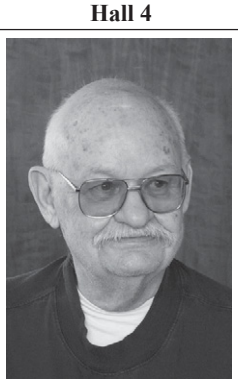
MOG pm 3:10 **Phosphotyrosine Proteome Analysis of *E. coli* Strains Using High Resolution Fourier Transform Mass Spectrometry**; Raghothama Chaerkady[1, 2]; Jyoti Sharma[2]; Santosh Renuse[2]; Harrys Kishore J[1, 2]; Nandini Patankar[2]; Sneha Pinto[2]; Harsha HC[1, 2]; Min-Sik Kim[1]; Anne-Marie Hanssen[3]; James B. Kaper[3]; Akhilesh Pandey[1]; *[1]Institute of Genetic Med, Johns Hopkins University, Baltimore, MD; [2]Institute of Bioinformatics, Bangalore, India; [3]University of Maryland School of Medicine, Baltimore, MD*

MOG pm 3:30 **Phosphoproteomic Survey of *in vitro* Kinase Substrates and the Phosphorylation Motif**; Naoyuki Sugiyama[1]; Haruna Imamura[1]; Koichi Yokota[2]; Sumiko Ohnuma[1]; Mai Tsukaha[1]; Masaru Tomita[1]; Yasushi Ishihama[1]; *[1]IAB, Keio Univ., Tsuruoka, Japan; [2]Carna Biosciences Inc., Kobe, Japan*

MOG pm 3:50 **A Tissue-Specific Atlas of Protein Phosphorylation and Expression in the Mouse**; Edward Huttlin[1]; Mark Jedrychowski[1]; Josh Elias[2]; Tapasree Goswami[1]; Ramin Rad[1]; Judit Villen[1]; Wilhelm Haas[1]; Mathew Sowa[1]; Steven Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Stanford University, Stanford, CA*

MOG pm 4:10 **Multiplexed Quantitative Analysis of the Differentiating Human ES Cell Phosphoproteome via High Mass Accuracy Tandem MS;** Nicole A Beauchene[1]; Danielle L Swaney[1]; Pengzhi Yu[1, 2]; Steven A Jackson[1, 2]; James A Thomson[1, 2]; Joshua J Coon[1]; *[1]University of Wisconsin, Madison, WI; [2]Morgridge Institute for Research, Madison, WI*

4:45 – 5:30 PM, MONDAY
AWARD LECTURE
Hall 4



Marvin L. Vestal, Recipient of the Award for a Distinguished Contribution in Mass Spectrometry

5:45 - 7:00 PM, MONDAY WORKSHOPS. *See page S7*

8:30 – 10:30 AM, TUESDAY MORNING
FUNDAMENTALS: BIOMOLECULAR ION-RADICAL CHEMISTRY
Frank Turecek, presiding
Room: Ballroom HJ

TOA am 08:30 **Evidence for Internal Energy Dependent Mechanisms in the Formation of Radical Product Ions in Electron Capture Dissociation**; Natalie Thompson; Daniel A. Thomas; Takashi Baba; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*

TOA am 08:50 **Tunable Fixed-Charge Tags for Electron Transfer Dissociation of Peptides**; Thomas W. Chung; Frantisek Turecek; *University of Washington, Seattle, WA*

TOA am 09:10 **Gas-Phase Structures of the Three-Helix Bundle Protein KIX Probed by Electron Capture Dissociation**; Martin Tollinger[2]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Austria; [2]Max F. Perutz Laboratories, Vienna, Austria*

TOA am 09:30 **Gas Phase Covalent Modification of Peptides via Ion/Ion Reactions: Schiff Base Formation on the Conversion of Ion Polarity**; Kerry Hassell; Scott A. Mcluckey; *Purdue University, West Lafayette, IN*

TOA am 09:50 **Elucidating Tertiary Structure in Gaseous Proteins Using Distant Dependent Hydrogen Atom Transfer between Radical Donor-Acceptor Pairs**; Tony Ly; Ryan R. Julian; *University of California, Riverside, Riverside, CA*

TOA am 10:10 **The dGdC Radical Cation Base Pair as a Model for Oxidative Damage in DNA**; Linda Feketeova[1]; Chan Bun[2]; George N. Khairallah[1]; Leo Radom[2]; Richard A. J. O'Hair[1]; *[1]Bio21 Inst & School of Chemistry,Uni of Melbourne, Melbourne, Australia; [2]School of Chemistry, University of Sydney, Sydney, Australia*

8:30 – 10:30 AM, TUESDAY MORNING
MS OF LIPIDS
Amina Woods, presiding
Room: Ballroom ACE

TOB am 08:30 **Novel Fragmentation Pathways Including Regioselective Attachment and Decompositions of Anionic Adducts of Steroids Formed by Electrospray Anion Attachment**; Nalaka Rannulu; Richard B. Cole; *University of New Orleans, New Orleans, LA*

TOB am 08:50 **Mitochondrial Lipid Profiling and Identification Using High Resolution LC-MS and MS/MS**; Susan Schiavo[1]; Vasant Marur[4]; Chunang (Christine) Gu [2]; Jules Phillips[3]; Bruce Kristal[5]; *[1]Brigham and Women's Hospital, Boston, MA; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, CA; [4]Brigham and Women's Hosp., Boston, MA; [5]Brigham + Women's Hospital, Boston, MA*

TOB am 09:10 **Localization, Imaging and Structural Analysis of Sialylated Glycosphingolipids in Brain Tissue Sections by Mass Spectrometry;** Benoit Colsch [1]; Shelley N. Jackson[1]; Sucharita M. Dutta[2]; Amina S. Woods[1]; *[1]NIDA-IRP, NIH, Baltimore, MD; [2]ThermoFisherScientific, San Jose, CA*

TOB am 09:30 **All Gunked Up and Nowhere to Flow: Profiles of Murine Atherosclerotic Plaques by High Spatial Resolution MALDI Imaging Mass**

Spectrometry; Peggi Angel; Kevin Tompkins; Kel Vin Woo; Scott Baldwin; Richard M. Caprioli; *Vanderbilt Univ Sch of Med, Nashville, TN*

TOB am 09:50 **Lipid Imaging by Matrix Implanted Laser Desorption/Ionization (MILDI) Ion Mobility-TOF MS Using Sub-Monolayer Nanoparticulate matrices**; J. Albert Schultz[1]; Ernest K. Lewis [1]; Thomas Egan[1]; Kelley Waters[1]; Valerie Vaughn[1]; Michael McCulley[1]; Jerry F. Moore[2]; Jeremy Post[3]; Alice Delvolve[3]; Amina S. Woods[3]; *[1]Ionwerks, Inc., Houston, TX; [2]MassThink LLC, Naperville, IL; [3]NIDA IRP, NIH, Baltimore, MD*

TOB am 10:10 **Identification of 1-Deoxy-Sphingoid Bases and *N*-Acyl-1-Deoxy-Sphingoid Bases by LC-ESI-MS/MS**; Hyejung Park[1]; Elaine Wang[2]; Mark Cameron Sullards[2]; Alfred H. Merrill[2]; Catherine E. Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]Georgia Institute of Technology, Atlanta, GA*

8:30 – 10:30 AM, TUESDAY MORNING
MS ON VIRUSES
Esther Van Duijn, presiding
Room: Ballroom BDF

TOC am 08:30 **Unravelling the Topology of Macromolecular Protein Complexes**; Alison E. Ashcroft; Tom W. Knapman; Victoria L. Morton; Peter G. Stockley; *University of Leeds, Leeds, UK*

TOC am 08:50 **Automated Limited Proteolysis and Intact Protein Hydrogen Exchange Reveals Mechanism of Action for a Novel Class of Anti-Hepatitis B Drugs**; Jonathan Hilmer[1]; Navid Movahed[1]; Adam Zlotnick[2]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT; [2]Indiana University, Bloomington, IN*

TOC am 09:10 **Virus Assembly and Stability Monitored by Native Electrospray and Ion Mobility Mass Spectrometry**; Glen Shoemaker[1]; Esther Van Duijn[1]; Sue Crawford[2]; Charlotte Uetrecht[1]; Marian Baclayon[3]; Wouter Roos[3]; Gijs Wuite[3]; Mary Estes[2]; Venkataram Prasad[2]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]Baylor College of Medicine, Houston, Texas; [3]Vrije Universiteit, Amsterdam, Netherlands*

TOC am 09:30 **High Throughput ESI-MS of PCR Products for the Identification of 2009 Pandemic Influenza A H1N1 Viruses;** Steven Hofstadler; Jared Drader; Jose Gutierrez; Ranga Sampath; Larry Blyn; David Ecker; *Ibis Biosciences, Inc., Carlsbad, CA*

TOC am 09:50 **Dynamic Evolution of the Macaque Pulmonary Proteome Response to Highly Pathogenic Avian Influenza and Spanish Flu Influenza Infections**; Joseph Brown[1]; Robert Palermo[2]; Jon Jacobs[1]; Marina Gritsenko[1]; Michael Katze[2]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratories, Richland, WA; [2]University of Washington - Dept. of Microbiology, Seattle, WA*

TOC am 10:10 **Identification of Host Cell Specific Markers in HIV Particles By Mass Spectrometry**; Lennard J.M. Dekker; Patrick H.M. Boers; Jeroen J.A. Van Kampen; Theo Marten Luider; Rob A. Gruters; *Erasmus Medical Center, Rotterdam, Netherlands*

8:30 – 10:30 AM, TUESDAY MORNING
MASS SPECTROMETRY OF PROTEIN-LIGAND COMPLEXES
Joseph Loo, presiding
Room 155

TOD am 08:30 **Quantifying Protein-Ligand Interactions with Electrospray Ionization Mass Spectrometry**; Elena Kitova[1]; Lan Liu[1]; Lu Deng[1]; Nian Sun[1]; Amr El-Hawiet[1]; Dhanashri Bagal [2]; Paul Schnier[2]; John Klassen[1]; *[1]University of Alberta, Edmonton, Canada; [2]Amgen, Thousand Oaks, CA*

TOD am 08:50 **High-Throughput Fragment Screening by Non-Covalent Mass Spectrometry;** Hannah Maple[1, 3]; Rachel Garlish[1, 2]; Matthew Crump[1, 3]; John Crosby[1, 3]; Richard Taylor[1, 2]; *[1], Bristol, UK; [2]UCB, Slough, Berkshire, UK; [3]School of Chemistry, University of Bristol, Bristol, UK*

TOD am 09:10 **Probing the Sites of Molecular Tweezer Noncovalent Binding to Amyloid β-Protein Using Top-Down ECD-FT-ICR MS**; Eric Pang[1, 2]; Sheng Yin[1]; Gal Bitan[2]; Thomas Schrader[3]; Joseph A. Loo[1]; David Teplow[2]; *[1]Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA; [2]Department of Neurology, UCLA, Los Angeles, CA; [3]University of Duisburg-Essen, Essen, Germany*

TOD am 09:30 **Characterization of Metal Coordinated Protein-Carbohydrate Complex Conformations via Ion Moblity-Mass Spectrometry**; Youjin Seo; Julie A. Leary; *UC Davis, Davis, CA*

TOD am 09:50 **Investigating Protein-Peptide Binding by 'Top-Down' FT-ICR MS, Ion-Mobility MS and Hydrogen/Deuterium Exchange;** David J Clarke[1]; Euan Murray[2]; Peter A Faull[2]; Ted Hupp[2]; Perdita Barran[2]; Pat Langridge-Smith[1]; C. Logan Mackay[1]; *[1]SIRCAMS, University of Edinburgh, Edinburgh, UK; [2]The University of Edinburgh, Edinburgh, UK*

TOD am 10:10 **Characterizing Cooperative Ligand Binding to Large Protein Complexes**; Liat Shimon; Amnon Horovitz; Michal Sharon; *Weizmann Institute of Science, Rehovot, Israel*

8:30 – 10:30 AM, TUESDAY MORNING
INCURRED SAMPLE REANALYSIS AND ANALYTICAL SOLUTIONS
Chengwei Fang, presiding
Room: Hall 2

TOE am 08:30 **Beyond Successful ISR: Case by Case Investigations for Unmatched Reassay Results When ISR Passed**; Robert Massé; Aimin Tan; Sylvain Lachance; Sofi Gagnon-Carignan; Ann Levesque; *Anapharm Inc., Quebec, QC*

TOE am 08:50 **Identifying Trends and Improving Outcomes from Incurred Sample Analysis Failure Investigations in a Bioanalytical CRO**; Patrick Bennett; Min Meng; Scott Reuschel; *Tandem Labs, Salt Lake City, UT*

TOE am 09:10 **Incurred Sample Reanalysis by a Bioanalytical Data Management System**; Joel I Usansky; Mike Small; Marc Krug; *Thermo Fisher, Philadelphia, PA*

TOE am 09:30 **Unexpected Event Investigation and Resolution for an ISR Test Failure for a SN-38 Assay Supporting a Clinical Study**; Qin C. Ji; Lisa Iacono; Dennis Garner; Mark E. Arnold; *Bristol-Myers Squibb Co., Princeton, NJ*

TOE am 09:50 **Application of Dried Blood Spots for the Analysis of a Novel Compound in the Presence of Liable Phase II Metabolites**; Hermes Licea Perez; Sharon Boram; Christopher Evans; *Bioanalysis, King of Prussia, PA*

TOE am 10:10 **The Evolution and Optimization of a High-Throughput LC/MS/MS Bioanalytical Method: HPLC-MS/MS vs. UFLC-MS/MS vs. UPLC-MS/MS**; Lisa Ford; Mike Allen; Kelli Goodman; *Enthalpy Analytical, Inc., Durham, NC*

8:30 – 10:30 AM, TUESDAY MORNING
QUANTITATION OF XENOBIOTIC METABOLITES WITHOUT REFERENCE STANDARD
Anne Aubry, presiding
Room: Hall 3

TOF am 08:30 **Estimation of Metabolite Concentrations in the Absence of an Authentic Standard Based on Relative $^{12}C/^{14}C$ Ratios Analyzed by High-Resolution ESI-MS**; Filip Cuyckens; Nadine Pauwels; Valerie Koppen; Laurent Leclercq; *Johnson & Johnson Pharma R&D, Beerse, Belgium*

TOF am 08:50 **A Novel Detection Technology Charged Aerosol Detection Coupled with HPLC, UV and LTQ Orbitrap MS for Drug Metabolism Study**; Hong Cai[1]; Jonathan L. Josephs [1]; Ragu Ramanathan[1]; Christopher Crafts[2]; Bruce A. Bailey[2]; William G. Humphreys[1]; *[1]Bristol-Myers Squibb, Pennington, NJ; [2]Dionex, Sunnyvale, CA*

TOF am 09:10 **Identification and Quantification of Reactive Metabolites and Their Adducts Using Electrochemistry Coupled to LC-MS**; Uwe Karst[1]; Wiebke Lohmann[1]; Anne Baumann[1]; Sandra Jahn[1]; Björn Meermann[1]; *[1]University of Münster, Münster, Germany*

TOF am 09:30 **LC-CaptiveSpray Ionization-Mass Spectrometry for Detection, Characterization and Quantification of Circulating Human Metabolites**; Nirmala Raghavan; Ragu Ramanathan; S. Nilgun Comezoglu; William Humphreys; *Bristol-Myers Squibb, Princeton, NJ*

TOF am 09:50 **The Performance of Accelerator Mass Spectrometry (AMS) for the Determination of 14C/C Isotope Ratios Using a Newly Installed BioMICADAS AMS**; Brad D. Keck; Pete Lohstroh; Jason Giacomo; John Vogel; *Vitalea Science, Inc., Davis, CA*

TOF am 10:10 **UPLC – ESI MSMS/ICPMS: A Tandem Tool for Quantitative Fingerprinting of Seleno-Metabolic Compounds**; Johann Far; Kasia Bierla; Brice Bouyssiere; Hugues Preud'homme; Ryszard Lobinski; *LCABIE - UMR5254 - IPREM, University of Pau, PAU, France*

8:30 – 10:30 AM, TUESDAY MORNING
QUANTITATION IN PROTEOMICS - PEPTIDES
Michael Washburn, presiding
Room: Hall 4

TOG am 08:30 **Experimental and Computational Strategies in Quantitative Proteomics**; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*

TOG am 08:50 **Minimally Permutated Peptide Analogs (MIPA) as Internal Standards for Relative and Absolute Quantification of Peptides and Proteins**; Joerg Seidler[1]; Dominic Winter[1]; Dominik Kugelstadt[2]; Bianca Derrer[2]; Barbara Kappes[2]; Wolf D. Lehmann[1]; *[1]German Cancer Research Center, Heidelberg, Germany; [2]University of Heidelberg, Heidelberg, Germany*

TOG am 09:10 **Spectral Counting Error Statistics from Nine Replicate MudPIT Samples**; Bret Cooper; *USDA-ARS, Beltsville, MD*

TOG am 09:30 **EtEP - A Novel Method to Produce an Equimolar Mixture of Standard Peptides for Absolute Quantification and Stoichiometry Determination**; Johann Holzmann[1]; Johannes Fuchs[1]; Otto Hudecz[2]; Peter Pichler[3]; Mathias Madalinski[1]; Robert Kurzbauer[1]; Karl Mechtler[1, 2]; *[1]Research Institute of Molecular Pathology, Vienna, Austria; [2]Institute of Molecular Biotechnology, Vienna, Austria; [3]Christian Doppler Laboratory for Proteome Analysis, Vienna, Austria*

TOG am 09:50 **Detection and Correction of Interference in MRM Analysis**; David Fenyo[1]; Sofia Waldemarson[2]; Guoan Zhang[2]; Asa Wahlander[2]; Beatrix Ueberheide[1]; Sunnie Myung[1]; Brian Reed[1]; Kelly Molloy[1]; Julio Cesar Padovan[1]; Jan Eriksson[3]; Thomas Neubert[2]; Brian Chait[1]; *[1]The Rockefeller University, New York, NY; [2]New York University Medical Center, New York, NY; [3]Swedish University of Agricultural Sciences, Uppsala, Sweden*

TOG am 10:10 **Development and Application of a System Suitability Standard and Protocol to Assess Data Quality in LC-MRM-MS across Multiple MS Platforms**; Susan E. Abbatiello[1]; Birgit Schilling[2]; D. R. Mani[4]; Xingdong Feng[8]; Lisa Zimmerman [6]; Brendan Maclean[5]; Michael P. Cusazk[2]; Terri Addona[1]; Nell Sedransk[8]; Michael J. Maccoss[5]; Steven C. Hall[3]; Steven A. Carr[1]; CPTAC Network[7; 1]*Broad Institute, Cambridge, MA; [2]Buck Institute for Age Research, Novato, CA; [3]UCSF Sandler-Moore Mass Spectrometry Core Facility, San Francisco, CA; [4]The Broad Institute of MIT and Harvard, Cambridge, MA; [5]University of Washington, Seattle, WA; [6]Vanderbilt University, Nashville, TN; [7]National Cancer Institute, Bethesda, MD; [8]NISS, Research Triangle Park, NC*

10:30 AM – 2:30 PM, TUESDAY
POSTER SESSION
Exhibit Hall ABCDE

2:30 – 4:30 PM, TUESDAY AFTERNOON
FUNDAMENTALS: ION SPECTROSCOPY
Mary Rodgers, presiding
Room: Ballroom HJ

TOA pm 2:30 **Alkali Metal Cationized Aliphatic Amino Acids: Charge-Solvation Becomes More Favorable with Increasing Ion Size**; Jos Oomens[1, 2]; Miriam Drayss[3]; Peter B. Armentrout[4]; Mathias Schaefer[3]; *[1]FOM Rijnhuizen, Nieuwegein, Netherlands; [2]University of Amsterdam, Amsterdam, Netherlands; [3]Inst. Organic Chemistry University of Cologne, Koeln, Germany; [4]University of Utah, Salt Lake City, UT*

TOA pm 2:50 **Gas Phase Structure of Micro-Hydrated Manganese Perchlorate Salts Probed by Infrared Spectroscopy**; Philippe Maitre[1]; Edith Nicol[1, 2]; Vincent Steinmetz[1]; Rajeev Sinha[1]; *[1]Laboratoire de Chimie Physique, Orsay, France;*